Fallo mecánico debido a grietas en Niobato de Litio bajo irradiación, simulación mediante elementos finitos

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PROGRAMA

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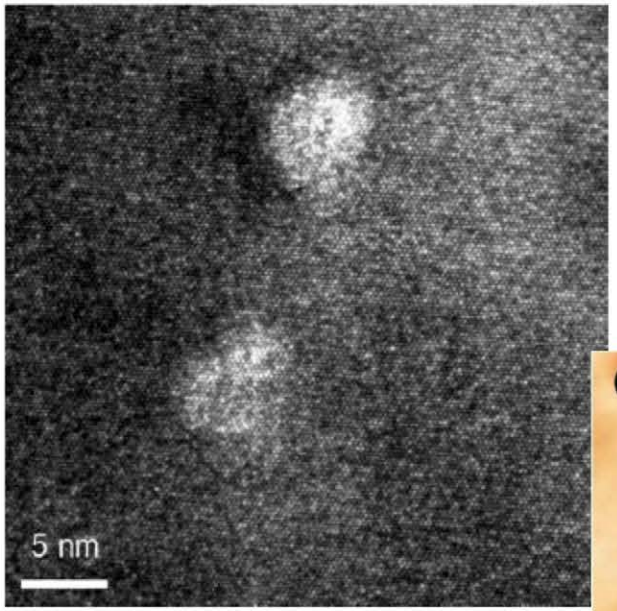
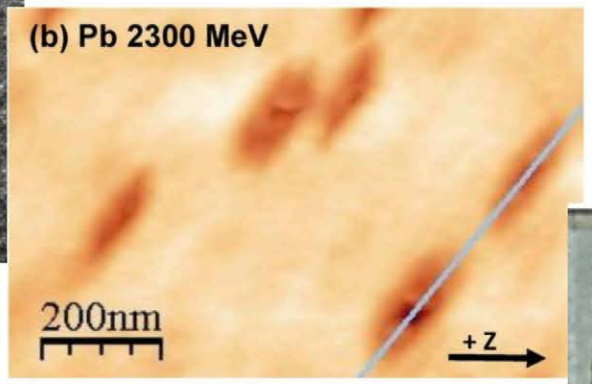
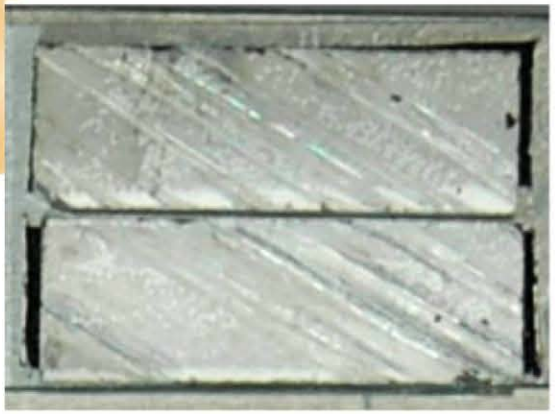
Ion-induced nano-tracks in LiNbO3



Swift heavy ions exceding MeV/amu produce columnar nano-tracks around the straight ion trajectory, with marked modifications with respect to the virgin material.



Crespillo et al. 2011
Rivera et al. 2011

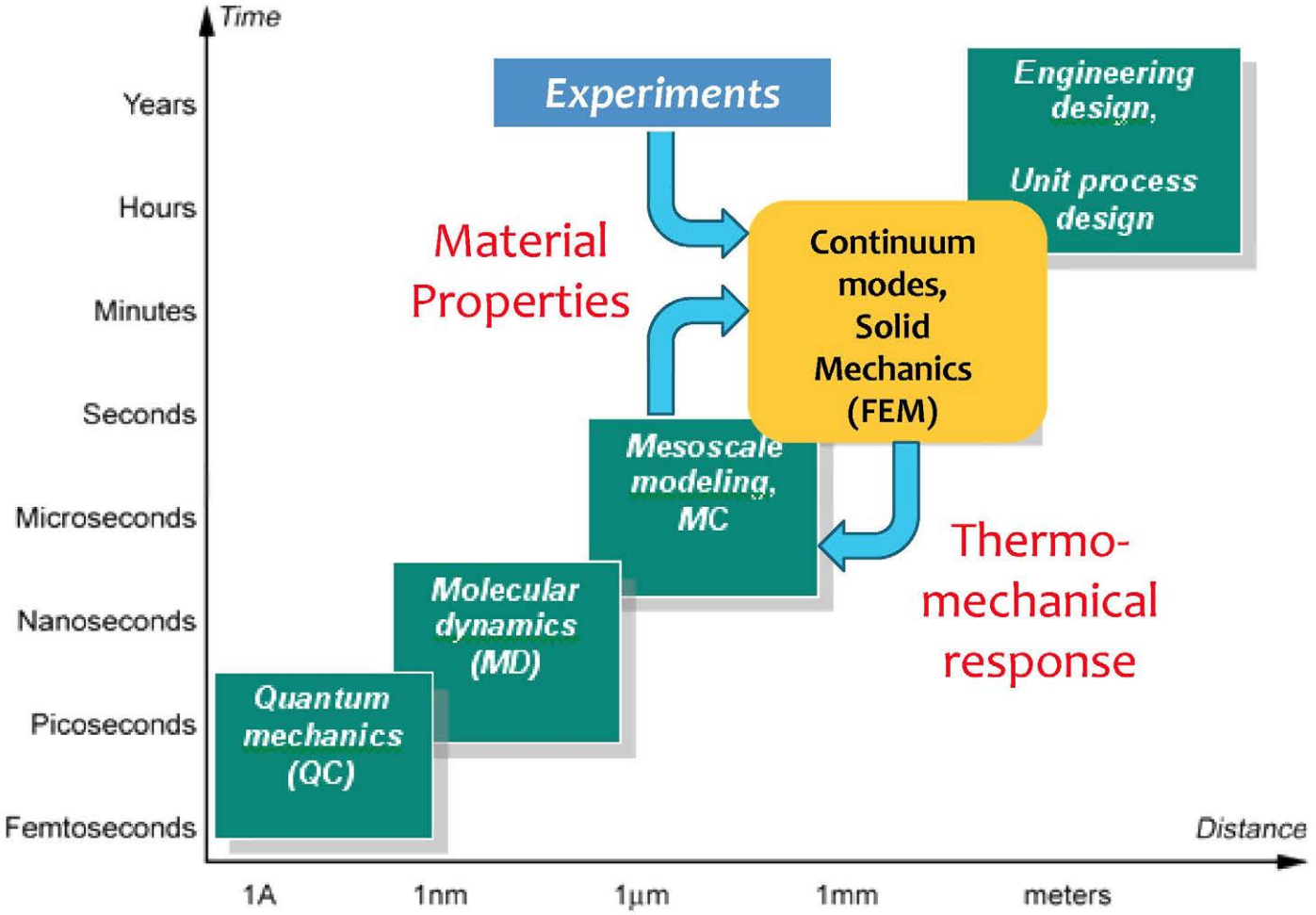


X

X

High fluence induces cracks (macroscopic effect)

From macro to nano-scale

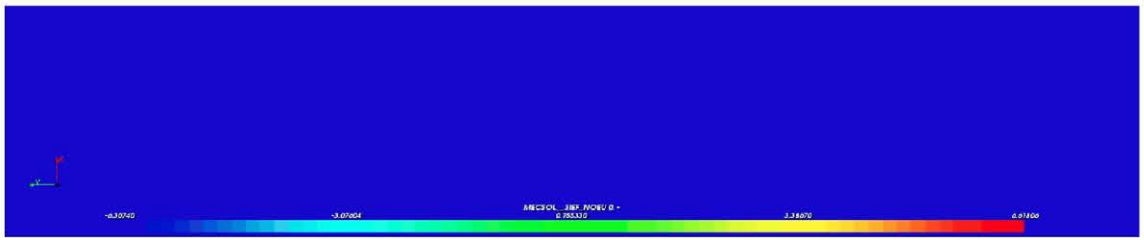


http://www.kintechlab.com/solutions/methodology/

Thermal spike

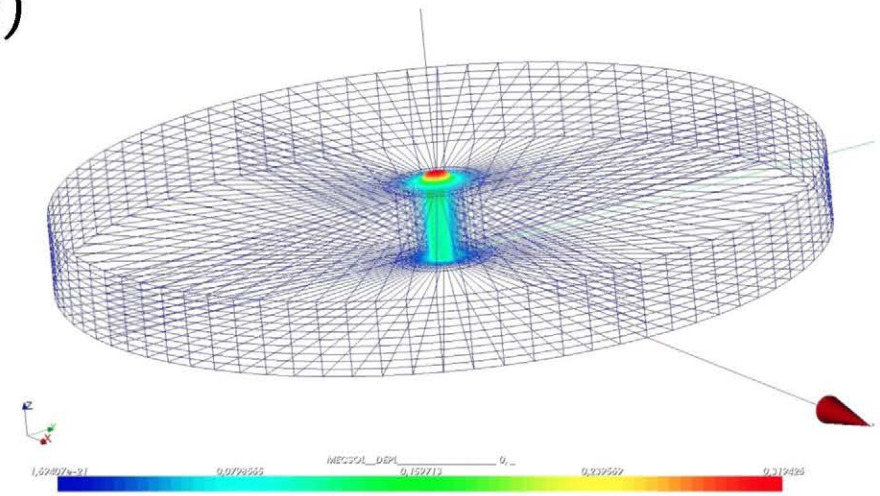
- Deposited energy heat the nano-track over fusion temperature
- The cooling left an amorphous nano-track with lower density
- The dilatation of nano-track induce deformations and stresses
- A hillock per nano-track are expected at surface

6 nm radius nano-track with stress in Y direction.

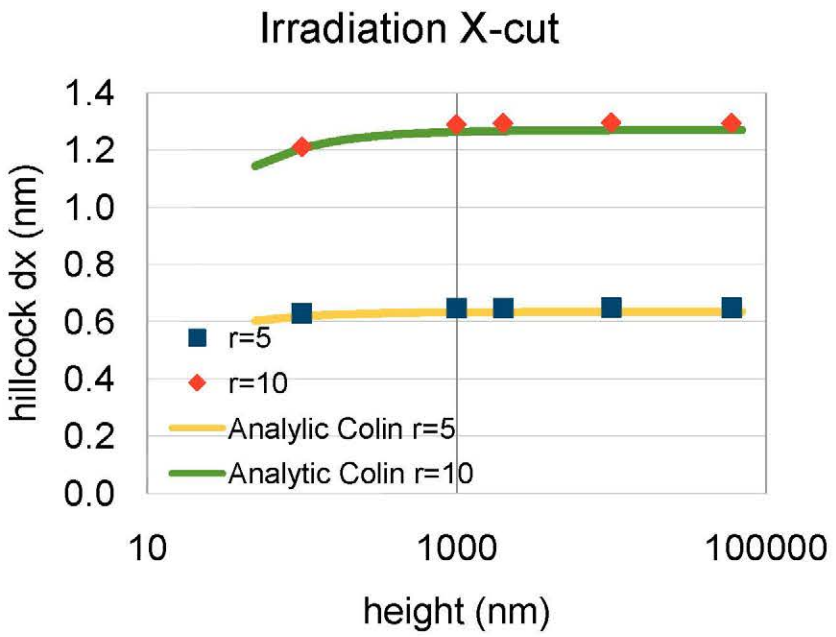


Finite element method for nano-structured materials

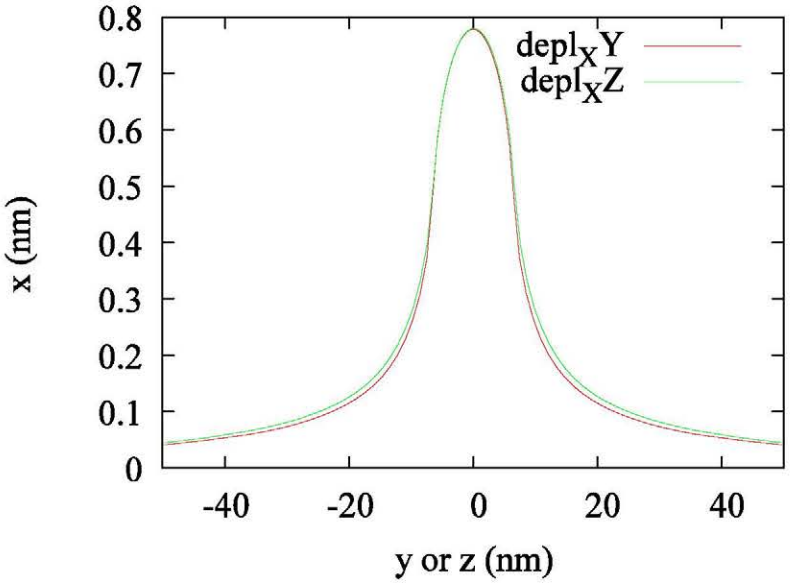
- Geometry simple but with huge range scales
- Orthotropic properties in crystal LiNbO3, and isotropic properties in amorphous track
- Boundary condition to simulate single track or multiple track (high fluence)



Simulations of X-cut in LiNbO3

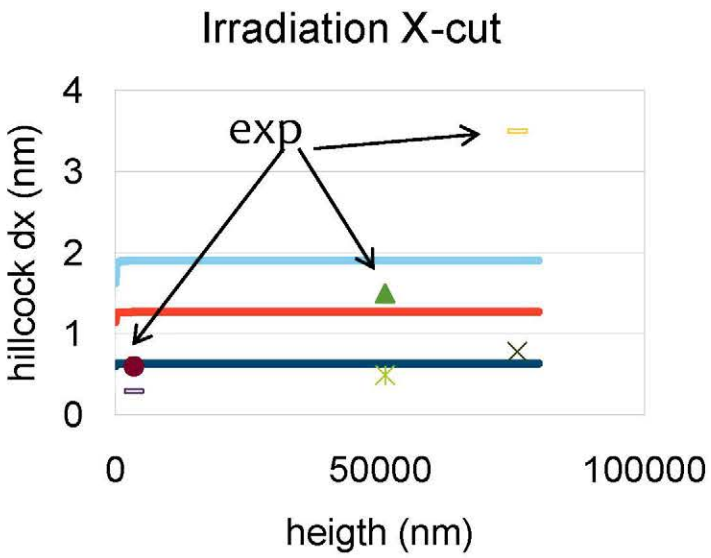


Simulations agree with analytical solution Colin et al. 2009



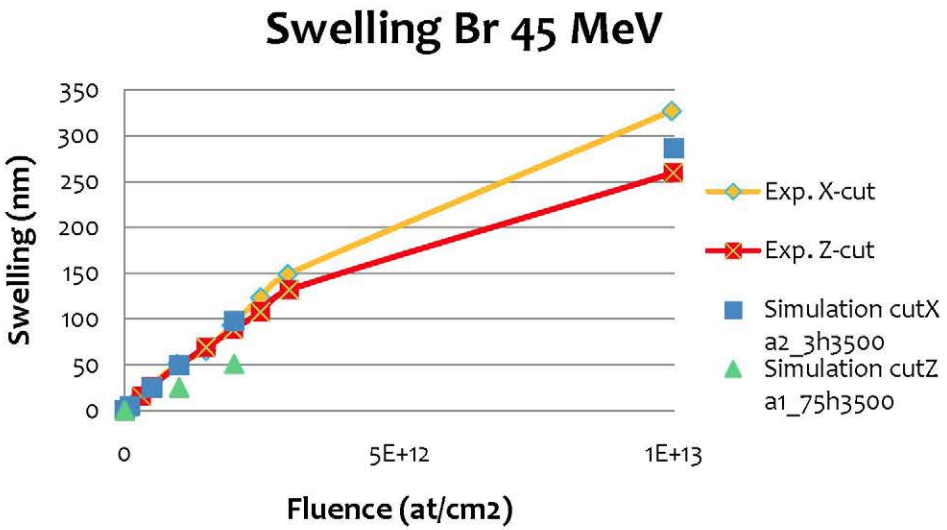
Hillcock has an elliptic shape due to orthotropic properties

Experiments versus simulations

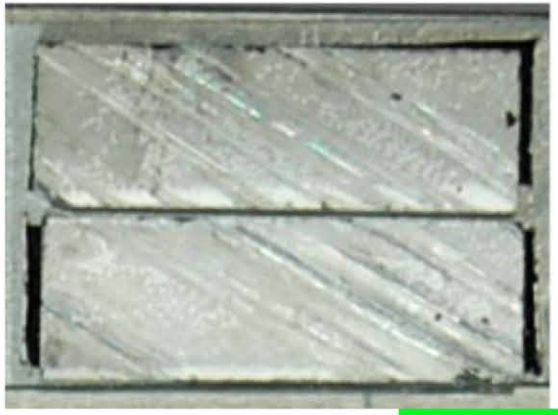


Experimental values of hillcocks are over the simulation ones.

X-cut swelling simulations agree with experimental data at low fluences.

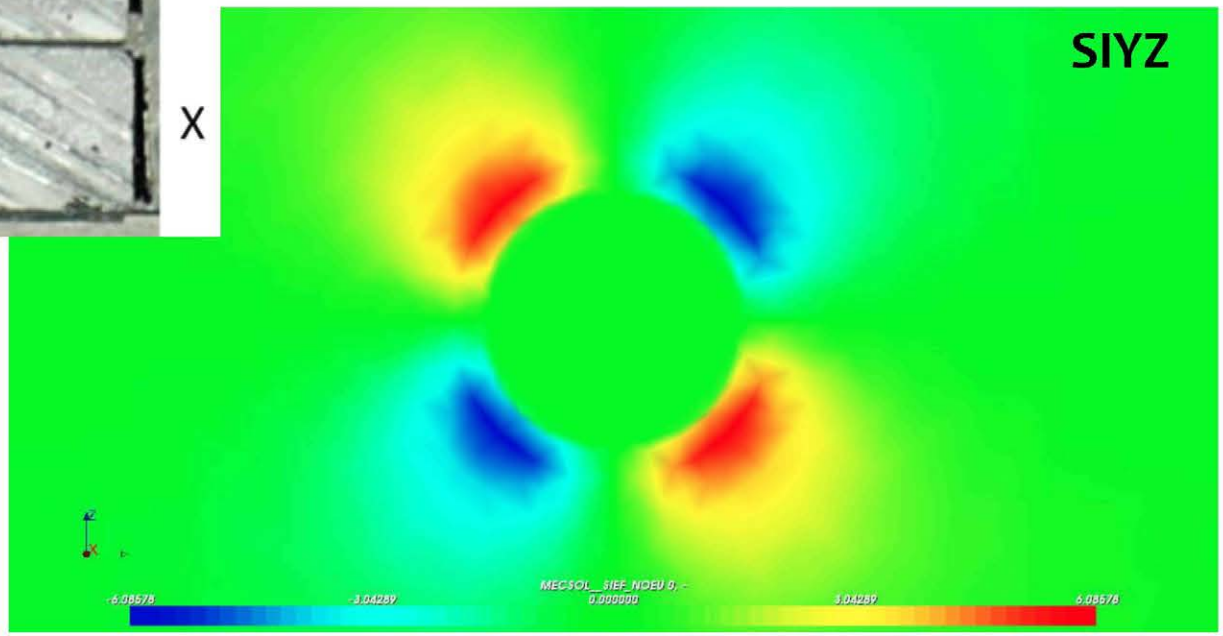


Cracks in X-cut



X Cracks for fluence > 2 10^{11}

X



Preference direction ±45°

Conclusions

- ✓ Finite elements can be used in nano-scale to fill the gap between theory and experiments.
- ✓ The elastic model must be complemented with plasticization to complete the ion-induce nano-tracks problem.

Thank you
Gracias